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Scientific Paper

Reuse of pulverized activated carbon for removing pesticides from water: potentials and limitations

Reúso de carvão ativado pulverizado para remoção de pesticidas da água: potenciais e limitações

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ABSTRACT

Pulverized activated carbon (PAC) adsorption is an effective complementary technique for removing pesticides in conventional water treatment. However, the high cost and residue generation associated with PAC use are significant drawbacks. This study evaluates the adsorption and desorption performance of atrazine (ATZ), simazine (SMZ), and diuron (DIU) using magnetized pulverized activated carbon (PACmag) for potential reuse in water treatment plants (WTPs). PAC16mag was identified as the adsorbent with the highest adsorption and desorption efficiencies. Under extreme contamination conditions, the process achieved removal efficiencies of 49.5% for ATZ, 53.8% for SMZ, and 69.1% for DIU, corresponding to residual concentrations of 712.9 μg L^{-1}, 572.6 μg L^{-1}, and 7,254.2 μg L^{-1}, respectively, from initial concentrations of 1,411.1 μg L^{-1}, 1,240.2 μg L^{-1}, and 23,410.4 μg L^{-1}. Kinetic studies revealed that the Elovich model best describes the adsorption process, highlighting heterogeneous surface interactions. Adsorption isotherms indicated that the Sips model provided the best fit, particularly for DIU, suggesting multilayer adsorption. The point of zero charge (pH_{PZC}) of PAC16mag was determined to be 7.1, indicating a near-neutral surface charge that facilitates adsorption through hydrophobic and π–π interactions. The desorption process reached 100%, with methanol (MeOH) exhibiting the best desorption efficiency. Although the magnetization process reduces PAC porosity indices, Fourier-transform infrared spectroscopy (FTIR) analyses revealed that Fe–O functional groups from magnetization enhance adsorptive efficiencies and facilitate material recovery. These findings suggest that magnetization is a promising technique for improving PAC performance and enabling its regeneration for reuse in WTPs.

Keywords: water treatment; pesticides; adsorption; desorption; pulverized activated carbon; magnetic adsorbents.

RESUMO

A adsorção por carvão ativado pulverizado (PAC) é uma técnica complementar eficaz para a remoção de pesticidas em tratamentos convencionais de água. No entanto, o alto custo e a geração de resíduos associados ao uso do PAC representam desvantagens significativas. Este estudo avalia o desempenho de adsorção e dessorção da Atrazina (ATZ), Simazina (SMZ) e Diuron (DIU) utilizando Carvão Ativado Pulverizado Magnético (PACmag), visando seu potencial reuso em Estações de Tratamento de Água (ETAs). O PAC16mag foi identificado como o adsorvedor com maiores eficiências de adsorção e dessorção. Em condições extremas de contaminação, o processo alcançou eficiências de remoção de 49,5% para ATZ, 53,8% para SMZ e 69,1% para DIU, correspondendo a concentrações residuais de 712,9 μg L^{-1}, 572,6 μg L^{-1} e 7.254,2 μg L^{-1}, respectivamente, a partir de concentrações iniciais de 1.411,1 μg L^{-1}, 1.240,2 μg L^{-1} e 23.410,4 μg L^{-1}. Estudos cinéticos revelaram que o modelo de Elovich descreve melhor o processo de adsorção, evidenciando interações heterogêneas na superfície. As isotermas de adsorção indicaram que o modelo de Sips apresentou o melhor ajuste, especialmente para o DIU, sugerindo adsorção em múltiplas camadas. O ponto de carga zero (pHPCZ) do PAC16mag foi determinado como 7,1, indicando uma carga superficial próxima à neutralidade, o que facilita a adsorção por interações hidrofóbicas e π-π. O processo de dessorção atingiu 100%, sendo o metanol (MeOH) o solvente com maior eficiência de dessorção. Embora o processo de magnetização reduza os índices de porosidade do PAC, análises de espectroscopia no infravermelho por transformada de Fourier (FTIR) revelaram que os grupos funcionais Fe-O oriundos da magnetização aumentam as eficiências adsortivas e facilitam a recuperação do material. Esses resultados sugerem que a magnetização é uma técnica promissora para aprimorar o desempenho do PAC e viabilizar sua regeneração para reuso em ETAs.

Palavras-chave: tratamento de água; pesticidas; adsorção; dessorção; carvão ativado pulverizado; adsorvedores magnéticos.

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INTRODUCTION

The intensification of agricultural activities to increase productivity, along with urban population growth, has recently contributed to environmental disturbances. The continuous introduction of pesticides, such as atrazine (ATZ), simazine (SMZ), and diuron (DIU), has polluted surface and underground water sources, especially in countries with extensive agricultural production (Barchanska et al., 2017; Chagas et al., 2019; Correia; Carbonari; Velini, 2020; Bachetti et al., 2021; García et al., 2022; Machado; Orrutéa; Panis, 2024; Xu et al., 2024).

The way these pesticides are used contributes to the contamination of aquatic environments. Hydrological transport phenomena, such as washing pesticide application equipment, crop runoff near rivers and lakes, irrigation, rainwater, and soil percolation, are involved in this process (Mandal; Singh; Purakayastha, 2017; Fang et al., 2025; Mendes et al., 2025; Zidan; Abdel-Halim; Eissa, 2025).

These contaminants can reach water treatment plants (WTPs) and are not effectively removed by conventional techniques (Francisco Fukumoto et al., 2022). This inefficacy occurs mainly because the pesticides are dissolved in low concentrations and have complex molecular structures (Sophia A.; Lima, 2018; Guo et al., 2022; Myers et al., 2022; Gomes et al., 2023; Wang et al., 2023; Gajendra et al., 2024; Peris et al., 2024; Quintero-Castañeda et al., 2024; Ali; Ali; Kombo, 2025; Mariappan et al., 2025). Consequently, they can enter the public water supply and pose risks to human health due to their bioaccumulative nature and toxicity, even at low concentrations, necessitating advanced water treatment techniques for their removal (Fröhlich; Foletto; Dotto, 2019; Pimenta et al., 2020; Zhou; Li; Achal, 2025).

Developing effective treatments for removing pesticides from supply waters has been the subject of many studies (Fuentes-López; Amézquita-Marroquín; Torres-Lozada, 2018; Ma; Arnold; Hozalski, 2018; Esquerdo et al., 2020; Pimenta et al., 2020; Assunção; Falda; Kuroda, 2023; Zeng et al., 2024; GokulaKrishnan et al., 2025; Imran; Ahmed, 2025; Kamel et al., 2025; Khan et al., 2025; Liu et al., 2025; Pal; Kioka, 2025; Pathiraja, 2025; Zhao et al., 2025). Adsorption is frequently used due to its high efficacy and simplicity of application on a real scale, especially when applied in powdered form (Chen et al., 2011; Francisco Fukumoto et al., 2022; Li et al., 2024), even in developing countries (Fuentes-López; Amézquita-Marroquín; Torres-Lozada, 2018; Pimenta et al., 2020).

Despite their high efficiency, PACs are costly and do not allow reuse in WTPs, making studies on their recovery and reuse necessary. Regenerating PACs is of great economic and environmental interest since they become waste after use in water treatment (Ledesma et al., 2015; Benhamed et al., 2016; Krause; Bronstein, 2024).

Several operational, analytical, and technological challenges are involved in reusing adsorbents. These challenges include separating/recovering used adsorbents in WTPs (Astuti et al., 2019) and employing efficient and sustainable techniques for desorbing the adsorbed analyses from the material. An important research area focus involves the modification of adsorbent composition and properties through magnetization, aiming to facilitate their separation and recovery from sludge while preserving their adsorption performance (Fröhlich; Foletto; Dotto, 2019; Nogueira et al., 2019; Ahmad et al., 2020; Azam et al., 2020; Rocha et al., 2020; Hadi et al., 2021; Drenkova-Tuhtan et al., 2024; Khalil et al., 2024; Nazempour et al., 2024).

This study aimed to evaluate the potentials and limitations of magnetized and non-magnetized PACs regarding their recovery and reuse after adsorbing ATZ, SMZ, and DIU, with a focus on optimizing conditions for practical application in WTPs. This included assessing the adsorption efficiency of the materials for these pesticides, determining the conditions and evaluating the desorption capacity to facilitate material reuse, selecting the most effective adsorbent based on its performance, and conducting a comparative analysis of the adsorbent's properties. To achieve this objective, a selection experiment for the carbon was conducted, followed by adsorption experiments to measure the removal capacity of the contaminants of interest from the study waters. Additionally, desorption experiments with different solvents were carried out to explore the possibility of reusing the selected PAC.

Given the limitations encountered in the present study, the following avenues for future research are suggested: (1) exploring the use of varied solvent volumes for elution assays to optimize the desorption process and enhance the efficiency of pollutant recovery; (2) investigating the impact of different pH levels on adsorption and desorption to gain deeper insights into the interactions occurring on the adsorbent surfaces; (3) evaluating the long-term reusability and regeneration methods for magnetized pulverized activated carbon (PACmag), along with assessing the associated costs and environmental impacts; (4) conducting experiments to measure the magnetic attraction force between magnetized carbon and magnets, and investigating the potential interference of different water matrices, such as raw water; and (5) conducting a study on solvent recovery during the desorption process to avoid mere phase transfer from one liquid to another, considering environmental concerns. Addressing these areas will improve the practical application of PACmag in water treatment processes and contribute to the development of more effective and sustainable approaches to contaminant removal.

METHOD

Analytical method and sample preparation

The pesticide detection and quantification were performed using an ultra-efficiency liquid chromatograph coupled with a photodiode array detector (UPLC-PDA) (Acquity H-Class, Waters), employing a C18 column (Acquity UPLC BEH C18 1.7 µm, 2.1×150 mm), at 40°C, with a mobile phase flow of 0.4 mL min^{-1} and a run temperature of 40°C. Ultrapure water acidified with 3 mmol phosphoric acid and high-performance liquid chromatography (HPLC)-grade acetonitrile (ACN) was used as the mobile phase in gradient mode. The retention times and wavelength determinations for each analysis were: ATZ (222 nm, 2.14 min), SMZ (222 nm, 3.73 min), and DIU (210 nm, 4.31 min) (Figure 1).

The analytical method was validated according to ANVISA (2017) and INMETRO (2020) guidelines, ensuring reliability (Table 1). Samples were collected at the specified times for each experiment, filtered, stored at -20°C, and analyzed to determine residual microcontaminant concentrations. For samples of ATZ (SD – Pestanal, CAS 1912-24-9, 99.1% purity; CP – Primatop SC), SMZ (SD – Pestanal, CAS 122-34-9, 99.9% purity; CP – Primatop SC), and DIU (SD – Pestanal, CAS 330-54-1, purity > 98%; CP – Herburon) with concentrations below the limit of quantification (LOQ), a solid-phase extraction (SPE) process was employed following methodologies adapted from (Montagner et al., 2014) and utilized by (Pimenta et al., 2020; Francisco Fukumoto et al., 2022), prior to further analysis by UPLC-PDA.

The linearity of the method was confirmed by determination coefficients (R^2) greater than 0.996 for all analytes, meeting the acceptance criterion of R^2

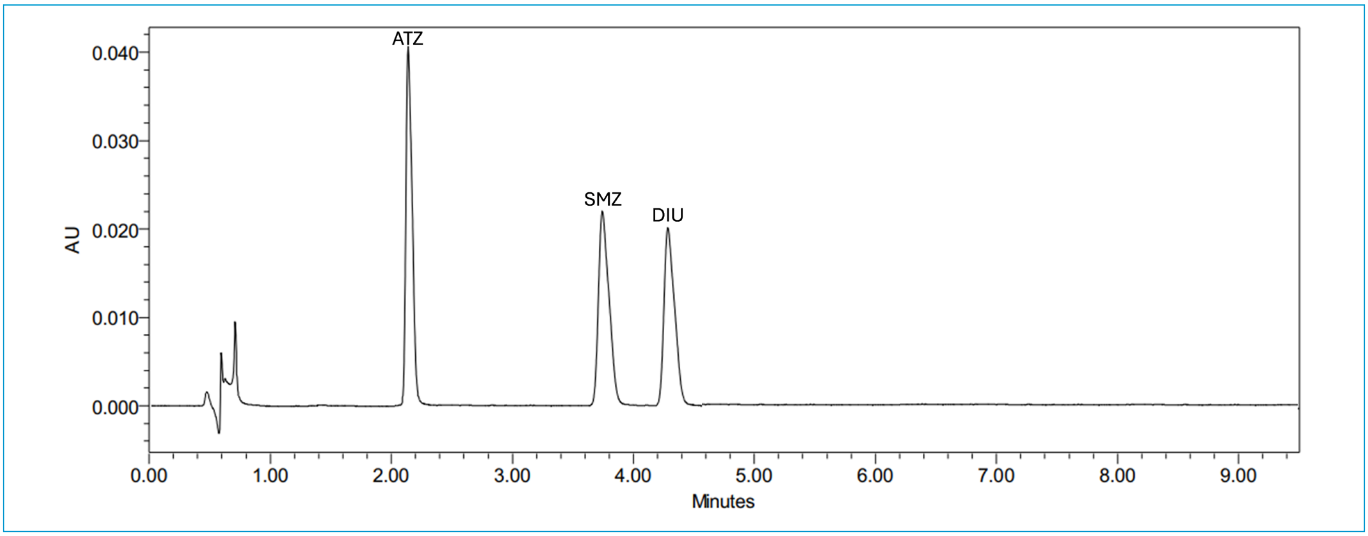


Figure 1 – Typical chromatogram of the pesticides obtained using the developed analytical method.

Table 1 – Method validation parameters of the compounds.

Compound	LOD	LOQ	Linearity	Recuperation (%)						Precision (%)	
	(µg L^{-1})	(µg L^{-1})	R^2	Ultrapure water		Treated water		Raw water		Intraday	Interday
				SD	CP	SD	CP	SD	CP		
ATZ	1.17	3.91	0.9998	97-99	83-107	112-94	101-104	87-103	103-111	5.46	7.91
SMZ	1.78	5.94	0.9998	112-117	87-110	77-107	102-108	95-116	101-110	11.10	13.01
DIU	1.88	6.28	0.9964	77-108	100-111	84-129	82-126	78-109	76-103	15.35	7.24

LOD: Limit of detection; LOQ: Limit of quantification; SD: Standard; CP: Commercial product.

≥ 0.99 (ANVISA, 2017). Recovery values ranged from 77 to 129%, depending on the analyte and matrix. According to INMETRO (2020), acceptable recovery values typically fall between 70 and 130%, although values slightly above this range (up to ~130%) can be accepted depending on matrix complexity and analyte level (Chiarello et al., 2023).

Water matrix composition

Synthetic waters (SWs) were prepared using ultrapure water fortified with commercial products (CPs) of ATZ, SMZ, and DIU to achieve concentrations that simulate extreme water contamination. These concentrations reflect the maximum values established in (Brasil, 2021), which stipulate the maximum permitted concentration of pesticides in water supplies in Brazil: 2 µg L-^{1} for ATZ-SMZ and 20 µg L-^{1} for DIU. Table 2 presents the physicochemical characteristics of the compounds.

Adsorbent material preparation and characterization

To enable the prospective analysis of the recovery of adsorbents, PAC5 and PAC16—provided by AlphaCarbo and Tobasa Bioindustrial, respectively—were magnetized (PAC5mag and PAC16mag) (Figure 2), with superparamagnetic iron oxide nanoparticles obtained by the thermo-decomposition, with a 5–10 nm range in diameter, resulting in stabilized material. The magnetization procedure was carried out in collaboration with the Laboratory of Supramolecular Chemistry and Nanotechnology (SisNano) at the University of São Paulo (USP), following a patented method (BR Patent BR1020140151397) (Nogueira et al., 2019). To maximize homogeneity and interaction between nanoparticles and activated carbon, both were suspended in cyclohexane at a ratio of 1:9 (nanoparticles:activated carbon). Subsequently, this mixture was heated, forming superparamagnetic composites (PACmag). For purification, magnetized PACs were washed with acetone (ACT) and dried at room temperature for later use.

The pulverized activated carbons (PACs) used in this study comply with the Brazilian standard NBR 12073:1991, which specifies that at least 95% of the material must pass through a mesh #325 sieve. Accordingly, both PAC5 and PAC16, before and after magnetization, exhibited similar particle size distributions, thereby ensuring consistency in this parameter across all samples evaluated.

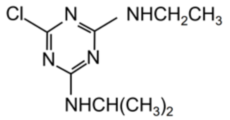
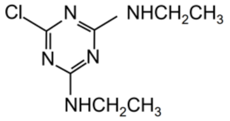
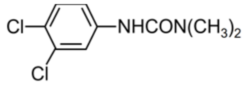
The materials were characterized by iodine number (IN) (NBR 12073/1991), methylene blue index (MBI), BET specific surface area (), and specific volume distribution of pore size, using gaseous nitrogen adsorption isotherms, with an analyzer for pore size distribution and specific surface area (model V-Sorb 2800P, Gold App Instruments).

The presence of superparamagnetic particles in PACmag and their attraction to a magnet (model N35, MagTek) can be observed in Figure 3.

Scanning electron microscopy

Scanning electron microscopy (SEM) was performed exploratively to complement the characterization of the selected adsorbent material and evaluate the adsorbent surface's morphological characteristics. Initially, the sample was coated with a 99.98% purity gold layer using a vaporizer (SCD 050, BAL-TEC), and 300 Å was deposited on the sample. Then, the sample was visualized by a scanning electron microscope (Quanta 200 model, FEI brand) coupled to the Oxford dispersive energy spectrometry system.

Table 2 – Selected physicochemical properties of the pesticides.

Compound	Chemical structure	Chemical formula	Molecular weight (g mol^{-1})	Size (Å)	Log K_{ow}
Atrazine		$C_8H_{14}ClN_5$	216.1	8.47	2.61
Simazine		$C_7H_{12}ClN_5$	202.0	7.5	2.18
Diuron		$C_9H_{10}Cl_2N_2O$	233.1	7.81	2.68

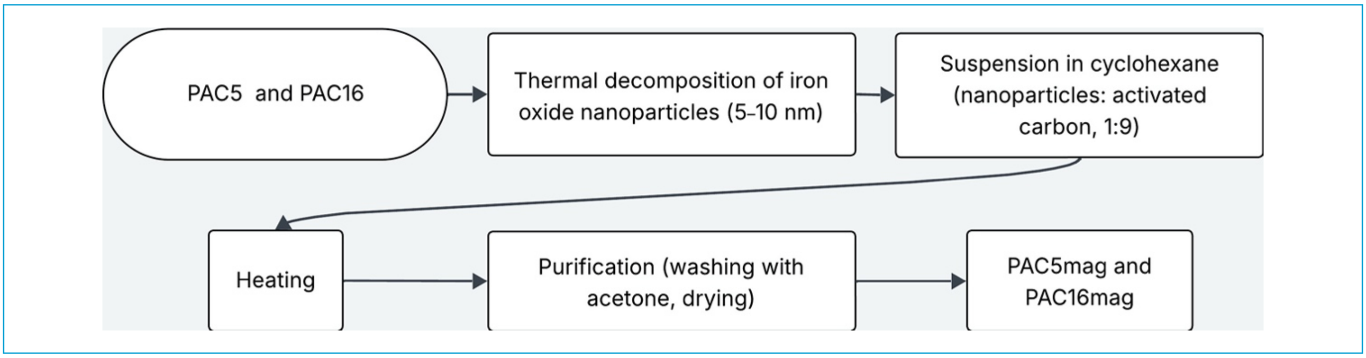


Figure 2 – Magnetization process.

Figure 3 – Magnetic attraction of PAC16mag compared to non-magnetic PAC16.

Fourier-transformed infrared with attenuated total reflectance analysis

To evaluate the functional groups present in the adsorptive materials, Fourier-transform infrared spectroscopy (FTIR) with attenuated total reflectance (ATR) was performed using a PerkinElmer FTIR spectrophotometer (USA) equipped with a diamond crystal supported by zinc selenide.

Following preliminary tests, the sample preparation method was established: drying the sample in an oven at 103°C for 24 h. Subsequently, PAC16mag was analyzed with atmospheric air as background. An aliquot of 100 µg of each sample was placed on the crystal, and 70 N torque was applied using an articulated arm. The spectrum was obtained at a resolution of 4 cm^{-1}, with 32 scans performed across the range of 500 to 4,000 cm^{-1}.

Adsorbent selection for pesticide removal based on adsorption efficiency

The PACs were dried in an oven at 103°C for 24 h and suspended in Sorensen's phosphate buffer (pH = 7.0) to minimize the influence of significant pH variations on adsorptive capacity. SW-1 (Table 3), composed of commercial ATZ, SMZ, and DIU products, was used at concentrations of 1 mg L^{-1} for ATZ and SMZ and 20 mg L^{-1} for DIU. Although ATZ, SMZ, and DIU are typically detected in surface waters at low concentrations, often in the order of ng L^{-1} to low µg L^{-1} (Sophia A.; Lima, 2018; Guo et al., 2022; Myers et al., 2022; Gomes et al., 2023; Wang et al., 2023; Gajendra et al., 2024; Peris et al., 2024; Quintero-Castañeda et al., 2024; Ali; Ali; Kombo, 2025; Mariappan et al., 2025), these elevated concentrations were chosen to simulate a scenario of extreme contamination of raw water, at levels significantly higher—500 and 1,000 times greater for triazines and DIU, respectively—than the maximum allowable values established by Ordinance GM/MS No. 888 of 2021 (Brazil, 2021).

The decision to adopt these high concentrations was further supported by preliminary adsorption assays, which demonstrated complete (or near-complete) removal of the pesticides when tested at lower concentrations. This total removal compromised analytical detectability and hindered the comparative evaluation of adsorbent performance. Thus, the selected concentrations aimed to ensure quantifiable residual levels after adsorption, allowing the effectiveness of the tested materials to be meaningfully distinguished.

The bench-scale experiment was conducted in amber glass flasks with a reaction volume of 100 mL, a PAC dosage of 100 mg L^{-1}, a pH of 7,0, and a contact time of 60 min, simulating application on a surface water catchment point.

Table 3 – Characteristics of synthetic waters used in experiments and concentrations obtained from CP from ATZ, SMZ, and DIU.

Notation	Synthetic matrix	Experiment	Pesticide concentration (µg L^{-1})		
			Atrazine	Simazine	Diuron
SW-1	Ultra-pure water	Adsorbent selection and desorption experiments	1,411.1	1,240.2	23,410.4
SW-2	Ultra-pure water	Isotherm	825.4	907.4	571.2
SW-3	Ultra-pure water	Kinetics	1,212.9	1,141.8	1,307.9

SW: Synthetic water

Contact time and point of application were determined based on the flow rate (2400 $L.s^{-1}$) of a WTP facility (operated by Paraná Sanitation Company – SANEPAR, situated in Londrina – PR/Brazil), aiming to determine the best conditions based on proper application parameters (Francisco Fukumoto et al., 2022). The experiment was agitated at 150 rpm and maintained at a temperature of 25°C ± 1°C in a shaker incubator (model NT 214, Nova Técnica).

The selected PAC concentration of 100 $mg \cdot L^{-1}$ was defined through preliminary tests, which indicated that higher dosages led to near-complete contaminant removal, potentially obscuring differences in performance between the evaluated adsorbents. Therefore, this intermediate dosage was chosen to preserve sensitivity in the comparison and ensure that distinctions in adsorption efficiency could be meaningfully assessed.

The agitation speed of 150 rpm was based on preliminary visual assessments, which identified this as the minimum rotational speed required to maintain complete and homogeneous mixing of the solid and liquid phases, without visible phase separation.

Adsorbent selection for pesticide removal based on desorption efficiency

Three HPLC-grade solvents were utilized for the recovery of adsorbent materials: methanol (MeOH – Honeywell), acetone (ACT – AppliChem), and acetonitrile (ACN – J. T. Baker). Following the adsorption experiment, the total reaction volume (SW+adsorbent) was filtered using a vacuum pump system (Tecnal model TE-058) through a 0.22 µm polyvinylidene fluoride (PVDF) membrane (Millipore) to separate non-magnetized adsorbents from the liquid medium. Magnetic separation of magnetized adsorbents was achieved using a neodymium magnet with a strength of 12,100 Gauss (model N35, MagTek). The retained mass of both non-magnetized and magnetized adsorbents was transferred to a 200 mL Erlenmeyer flask for the desorption experiment. Each reaction was conducted with the same volume of treatment sample of the respective solvent, followed by constant agitation at 150 rpm and a temperature of 25°C ± 1°C in a shaker incubator (model NT 214, Nova Técnica) for a contact time of 24 h.

Adsorption isotherms

The experiment was conducted following the guidelines of ASTM D 3860 (ASTM, 2003) with modifications. Glass bottles with a reaction volume of 70 mL and PAC dosages of 1, 2.5, 5, 10, 20, 30, 40, 50, and 60 mg L^{-1} were used under the same conditions as the selection experiment (Section 2.4), with samples collected every 3 h. SW-2 (Table 3) was prepared with commercial ATZ, SMZ, and DIU products, containing concentrations of 1 mg L^{-1} of ATZ and SMZ and 0.5 mg L^{-1} of DIU. The equilibrium time was determined when the difference between the residual concentrations of ATZ, SMZ, and DIU for each PAC dosage was less than 5% in consecutive analyses. The data were then adjusted to the Langmuir, Freundlich, Sips, and Redlich–Peterson isotherm models and then analyzed.

Adsorption kinetics

In the adsorption kinetic experiments, a dosage of 60 mg L^{-1} of PAC was added to a SW-3, with a reaction volume of 300 mL in 10 separate 500 mL Erlenmeyer flasks. The flasks were agitated under controlled conditions: agitated at 150 rpm and maintained at a temperature of 25°C ± 1°C in a shaker incubator (model NT 214, Nova Técnica), for predetermined contact times of 0, 5, 10, 15, 30, 60, 120, 180, 360, 720, and 1260 min. All experiments were performed in triplicate to ensure reproducibility.

The equilibrium time for adsorption utilized of 21 h was previously determined in the adsorption isotherm experiment (Section 2.6). After completing the kinetic tests, the experimental data were fitted to pseudo-first-order (PFO), pseudo-second-order (PSO), and Elovich kinetic adsorption models to evaluate the adsorption mechanisms. These models are widely employed to describe adsorption mechanisms, providing insights into the dominant processes in various systems (Lladó et al., 2015; Mandal; Singh; Purakayastha, 2017; Hadi et al., 2021).

Determination of the point of zero charge

The pH_{pzc} determination procedure involved adding 20 mg of the adsorbent to 20 mL of a 0.1 $mol \cdot L^{-1}$ NaCl aqueous solution, prepared at 12 different initial pH conditions (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and 12), adjusted with 0.1 $mol \cdot L^{-1}$ HCl or NaOH solutions. The mixtures were equilibrated for 24 h in a shaker incubator (model NT 214, Nova Técnica) at 25°C, under stirring at 100 rpm. After equilibration, the solutions were filtered, and the final pH values were measured. The pH_{PZC} was defined as the range in which the final pH remains constant regardless of the initial pH, indicating a buffering behavior of the adsorbent surface. All experiments were performed in triplicate.

RESULTS AND DISCUSSION

Characterization of adsorbent materials

The magnetization process resulted in a substantial reduction in the microporosity (IN) and mesoporosity (MBI) values of the adsorbents. Specifically, PAC5 exhibited reductions of 42 and 10% for IN and MBI, respectively, while PAC16 showed reductions of 40 and 14% for IN and MBI, respectively (Table 4).

Regarding specific surface area (BET area) and specific volume distribution as a function of pore size (Table 4), a similar reduction pattern was observed post-magnetization. The micropore surface area (BET) decreased by 31% for PAC5 compared to PAC5mag and by 44.5% for PAC16 compared to PAC16mag. Additionally, the micropore-specific volume reduced by 31% for PAC5 relative to PAC5mag and by 45% for PAC16 relative to PAC16mag. Conversely, the BET area and pore size-specific volume associated with macropores increased following the magnetization process.

These changes are primarily attributed to two factors related to the magnetization process. First, the reduction in micropores is likely due to the obstruction of their entry by superparamagnetic iron oxide nanoparticles (Nogueira et al., 2019; Drenkova-Tuhtan et al., 2024; Quintero-Castañeda et al., 2024; Ali; Ali; Kombo, 2025; Mariappan et al., 2025). Although these nanoparticles have diameters ranging from 5 to 10 nm, which are larger than the micropore diameters (< 2 nm), they can still obstruct the entry of micropores, as these are mainly formed within mesopores. Second, the magnetization process can create a layer of superparamagnetic iron oxide nanoparticles on the material's surface, which bonds with the carbon. Given the irregular surface of the PAC, the nanoparticles are randomly distributed post-magnetization, potentially forming a multilayer configuration at various points, leading to increased measurements of BET and specific volume of mesopores (Nogueira et al., 2019; Rocha et al., 2020; Drenkova-Tuhtan et al., 2024; Khalil et al., 2024; Nazempour et al., 2024; Pet et al., 2024).

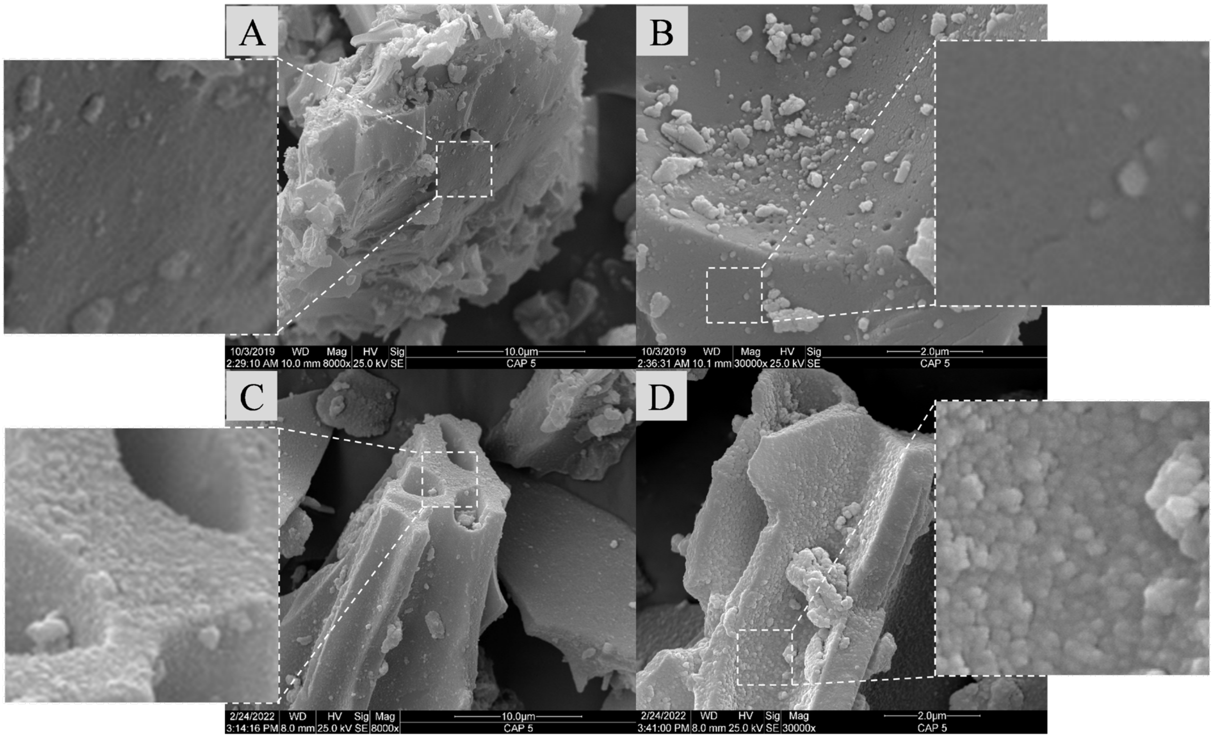
Scanning electron microscopy

SEM approximations of 8,000 and 30,000 times were made for all activated carbons to identify possible morphological changes in the surface due to their magnetization. It is observed that the surfaces of PACs before magnetization (Figures 4A, 4B, 5A, and 5B) are relatively smooth, whereas PAC5mag and PAC16mag (Figures 4C, 4D, 5C, and 5D) exhibit greater surface heterogeneity. This characteristic may be attributed to the impregnation of superparamagnetic nanoparticles, which formed a superficial layer in the activated carbons. This corroborates the assumption made previously, explaining the reduction in micropores and the increase in mesopores, as shown in Table 4. The surface coating of the activated carbons with magnetic nanoparticles observed in this study is consistent with findings reported in recent literature (Drenkova-Tuhtan et al., 2024; Khalil et al., 2024; Nazempour et al., 2024).

Table 4 – Properties and characterization of adsorbent materials concerning the origin, activation method, raw material, iodine number, and methylene blue index.

Name	Origin	Activation mode	Raw material	IN	MBI	Specific surface area – BET		Pore size specific volume	
						Micropore	Mesopore	Micropore	Mesopore
				(mg g^{-1})	(mg g^{-1})	(cm² g^{-1})	(cm² g^{-1})	(cm³ g^{-1})	(cm³ g^{-1})
PAC5	Vegetable	Physical	Pinus	942	134	609.9	267.8	0.250	0.297
PAC16	Vegetable	Physical	Babassu	780	112	735.15	109.85	0.312	0.116
PAC5mag	Vegetable	Physical	Pinus	549	121	370.45	302.37	0.172	0.344
PAC16mag	Vegetable	Physical	Babassu	468	96	386.09	173.29	0.173	0.203

IN: Iodine number; MBI: Methylene blue index; PAC: Pulverized activated carbon; PACmag: Magnetized pulverized activated carbon; NA: Not applicable.



A and C: 8000x approximation; B and D: 30000x approximation;
A and B: PAC5;
C and D: PAC5mag.

Figure 4 – PAC5 and PAC5mag micrographs obtained by SEM and details (5x zoom).

Fourier-transformed infrared with attenuated total reflectance analysis

To complement the characterization of the selected adsorbent materials, Fourier-transformed infrared spectra associated with total attenuated reflectance (FTIR/ATR) were obtained for PAC16 and PAC16mag prior to their *use* in adsorption experiments. These spectra aimed to assess changes induced by the magnetization process and potentially elucidate the discussed adsorption efficiencies. Figure 6 illustrates the FT-IR/ATR spectra for PAC16 and PAC16mag.

In both materials, distinct peaks were observed at wavelengths 2,680, 2,350, 2,130, 1,560, 1,085, and 870 cm^{-1}. The 2680 cm^{-1} band corresponds to C–H bond vibrations (e.g., -CH3 and -CH2) (Liu et al., 2020; Mandal et al., 2021). The peak at 2,350 cm^{-1} arises from alkyne group stretching and vibration, C≡C (Wang et al., 2010; Gupta et al., 2013). The band at 2,130 cm^{-1} relates to C=N vibration (Zhang et al., 2021), while the 1,560 cm^{-1} band indicates C=C bonds from alkene groups (Azam et al., 2020).

In the spectrum of PAC16mag, additional bands at 580–630 cm^{-1} signify superparamagnetic nanoparticles derived from Fe–O vibrations, confirming their integration into the activated carbon matrix (Bordbar et al., 2014; Azam et al., 2020; Saleh; Tuzen; Sari, 2017). Moreover, reductions in the intensity of prominent peaks (2,680, 2,350, 2,130, 1,560, and 1,085 cm^{-1}) in this material suggest surface modifications due to the presence of superparamagnetic nanoparticles.

The vibration of CH_2 groups (2,680 cm^{-1}) in both materials contributes to the enhanced efficiency observed in PAC16 and PAC16mag, as depicted in Figure 6. The presence of amine protons on the molecular surface enhances positive charges, thereby favoring adsorption (Pimenta et al., 2020).

Furthermore, the emergence of Fe–O oxygenated groups (580–630 cm^{-1}) in PAC16mag may explain its superior adsorption efficiency. These oxygenated groups increase electron density on the graphitic planes of activated carbon, where ATZ and SMZ, as π-deficient compounds with chlorine substituents acting as electron-withdrawing groups, exhibit affinity with the activated carbon (Lladó et al., 2015; Francisco Fukumoto et al., 2022). Additionally, ATZ, SMZ, and DIU can bind to the surface of magnetite nanoparticles, occupying vacant sites or substituting passivating ligands (Lladó et al., 2015; Francisco Fukumoto et al., 2022).

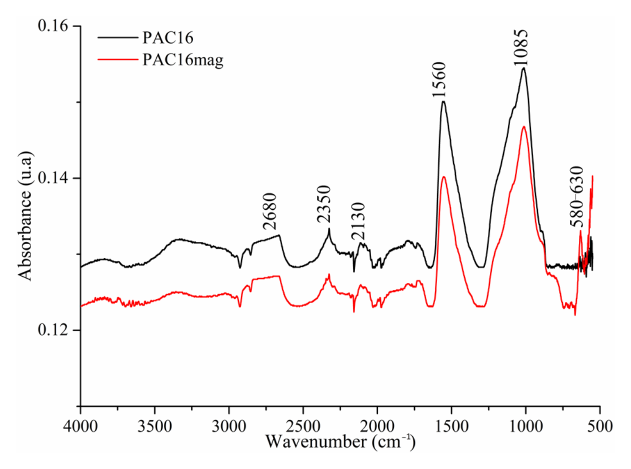
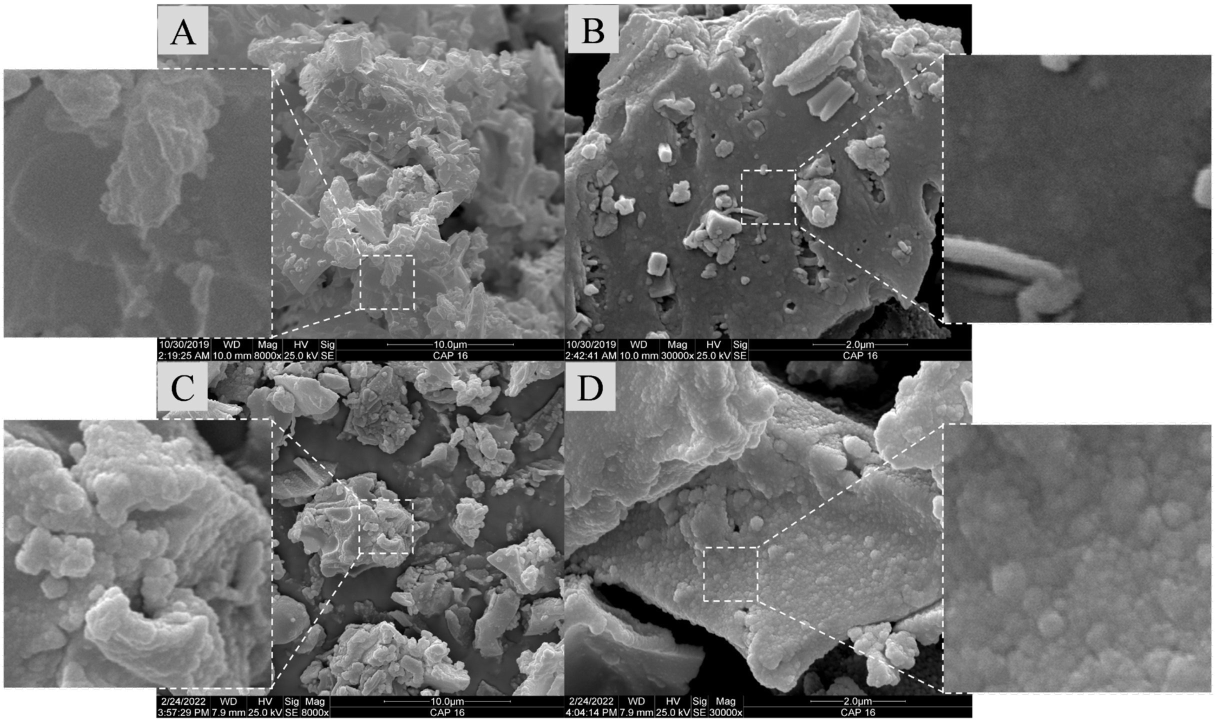


Figure 6 – FT-IR/ATR spectrum for PAC16 and PAC16mag. cm^{-1}cm^{-1}.



A and C: 8000x approximation; B and D: 30000x approximation;
A and B: PAC16;
C and D: PAC16mag.

Figure 5 – PAC16 and PAC16mag micrographs obtained by SEM and details (5x zoom).

Considering the interactions involving CH_2 and Fe–O groups and the behavior observed in pH_{PZC}, it can be concluded that the surface charge properties of PAC16mag, with a pH_{PZC} near pH 7, played a key role in the adsorption process. The presence of functional groups such as amines and oxygenated sites enhances the surface characteristics, promoting stronger interactions with pesticides. These interactions, combined with hydrophobic effects and the affinity of magnetite nanoparticles, help explain the observed adsorption order (DIU > ATZ > SMZ). Thus, the molecular structure and surface modifications of PAC16mag work in synergy, improving its ability to adsorb pesticides by optimizing both electrostatic and non-electrostatic interactions.

Adsorbent selection for pesticide removal based on adsorption efficiency

Analysis depicted in Figure 7 reveals that magnetized forms of PACs exhibited higher adsorptive efficiency compared to their original commercial forms, with enhancements ranging from 11.1 to 20.7%.

Under identical conditions of SW and adsorbent dosage, PAC16 demonstrated the highest removal efficiencies for pesticides ATZ, SMZ, and DIU at 29.2, 33.1, and 53.7%, respectively. Following magnetization, these removal efficiencies increased to 49.5, 53.8, and 69.1%, making PAC16mag the most effective PAC under these conditions.

Considering the characteristics of the materials employed in this study, as presented in Table 4, and the relatively small molecular masses of ATZ, SMZ, and DIU (216.1, 202.0, and 233.1 g mol^{-1}, respectively), it was expected that adsorbent materials with higher NI values would exhibit greater efficiencies in the removal of these pesticides. However, the data revealed that after magnetization, while adsorption efficiency increased, the characterization indices such as NI were significantly reduced, complicating the establishment of a clear correlation between material properties and removal efficiency.

Contrary to expectations, the magnetization process led to a reduction in micropore volume and area in PAC5mag and PAC16mag. Despite the small molecular sizes of ATZ, SMZ, and DIU (8.47 Å, 7.5 Å, and 7.81 Å, respectively) (Table 2), adsorption was anticipated to primarily occur in micropores. However, no direct correlation was observed between removal efficiencies and micropore volume or specific surface area (BET), suggesting that pore size and distribution do not significantly limit adsorption. Instead, physicochemical interactions such as hydrophobicity, polarity, π–π interactions, and hydrogen bonds likely govern the adsorption mechanisms (Lladó et al., 2015; Pimenta et al., 2020; Francisco Fukumoto et al., 2022).

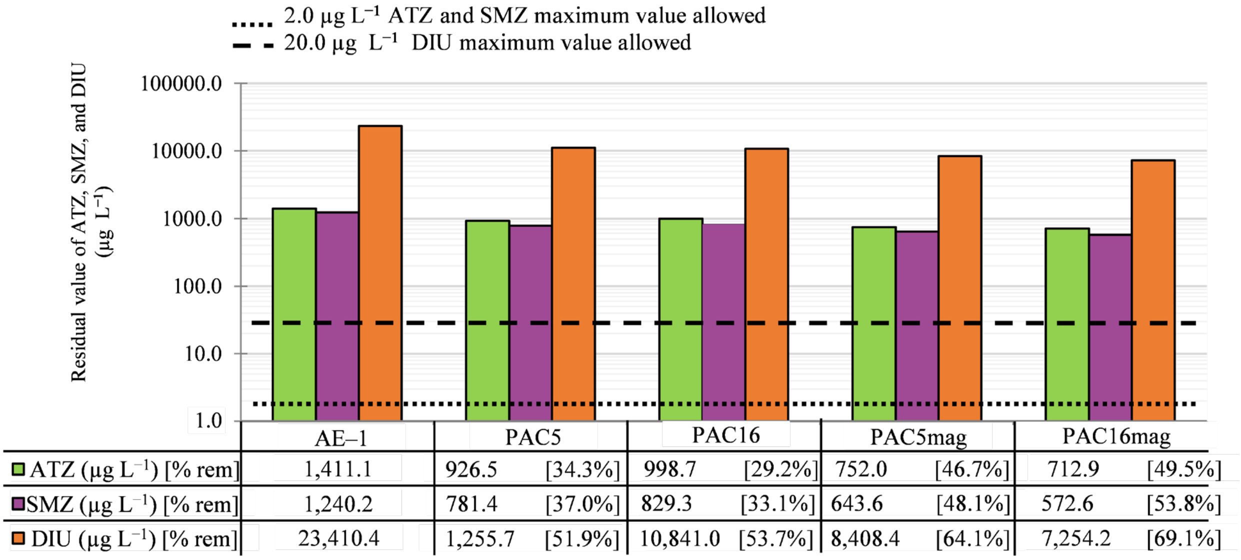
Overall, the pesticide removal efficiency followed the order: %DIU > %SMZ > %ATZ, attributed to the polarity of the molecules, with ATZ and SMZ being polar and DIU less so. In the adsorption process of organic compounds in water (a polar solvent) onto nonpolar materials (ACs), less polar compounds like DIU exhibit weaker attraction to the solvent and thus are more likely to adsorb onto nonpolar ACs (Snoeyink; Summers, 1990; Pimenta et al., 2020).

Log Kow values serve as preliminary indicators of adsorption affinity in activated carbon (Dhangar; Kumar, 2020; Lopes et al., 2020; Pimenta et al., 2020; Saleh; Zouari; Al-Ghouti, 2020; Tang et al., 2020; Campinas et al., 2021; Dong et al., 2021; Jatoi et al., 2021). The descending order of log Kow values was $\log_{KowDIU} > \log_{KowATZ} > \log_{KowSMZ}$, correlating with the removal percentages of %DIU > %SMZ > %ATZ. The minimal difference in removal rates between ATZ and SMZ (3.1%) supports the hypothesis that molecular polarity and hydrophobic interactions significantly influence adsorption onto PACs.

Moreover, the linear and flat structure of the DIU molecule, facilitated by electron relocation stiffening the urea part and aligning it with the phenyl group, enhances its transport to the active sites and pores of PACs. In contrast, the ethyl and isopropyl groups of ATZ and SMZ, which are not in the triazine plane due to steric hindrance, impart a less linear and more voluminous shape, potentially hindering their adsorption onto PACs (Rambabu et al., 2012; Pimenta et al., 2020; Francisco Fukumoto et al., 2022).

Adsorbent selection for pesticide removal based on desorption capacities

After the adsorption experiment, the masses were recovered, and recovery efficiencies ranging from 98 to 100% were achieved for both tested conditions (filtration and magnetic separation).



	AE–1	PAC5	PAC16	PAC5mag	PAC16mag
🟩 ATZ ($\mu g\ L^{-1}$) [% rem]	1,411.1	926.5 [34.3%]	998.7 [29.2%]	752.0 [46.7%]	712.9 [49.5%]
🟪 SMZ ($\mu g\ L^{-1}$) [% rem]	1,240.2	781.4 [37.0%]	829.3 [33.1%]	643.6 [48.1%]	572.6 [53.8%]
🟧 DIU ($\mu g\ L^{-1}$) [% rem]	23,410.4	1,255.7 [51.9%]	10,841.0 [53.7%]	8,408.4 [64.1%]	7,254.2 [69.1%]

Figure 7 – Residual concentration of the commercial product of SMZ, ATZ, and DIU after adsorption in PACs, and percentage removal.

After separating the activated carbon, the desorption experiments were conducted. For SMZ, the solvents used (MeOH, ACN, and ACT) were ineffective in analyte desorption for any adsorbent materials. Figure 8 demonstrates that, for the desorption of ATZ, ACT was more efficient than the other solvents for all adsorbents, except for PAC5mag and PAC16mag, where MeOH exhibited higher desorption performance, achieving 70.5 and 73.3%, respectively.

Regarding DIU (Figure 8), ACN and MeOH showed similar desorption efficiencies, with percentages ranging from 86 to 100%. Therefore, it can be observed that for magnetized PACs, which exhibited the highest adsorption efficiencies, MeOH and ACN demonstrated the highest desorption capacities for the analytes of interest.

The sum of the total masses of the desorbed analytes for each solvent and adsorbent is represented in Figure 9, where the best performance was observed for PAC16mag with the use of MeOH.

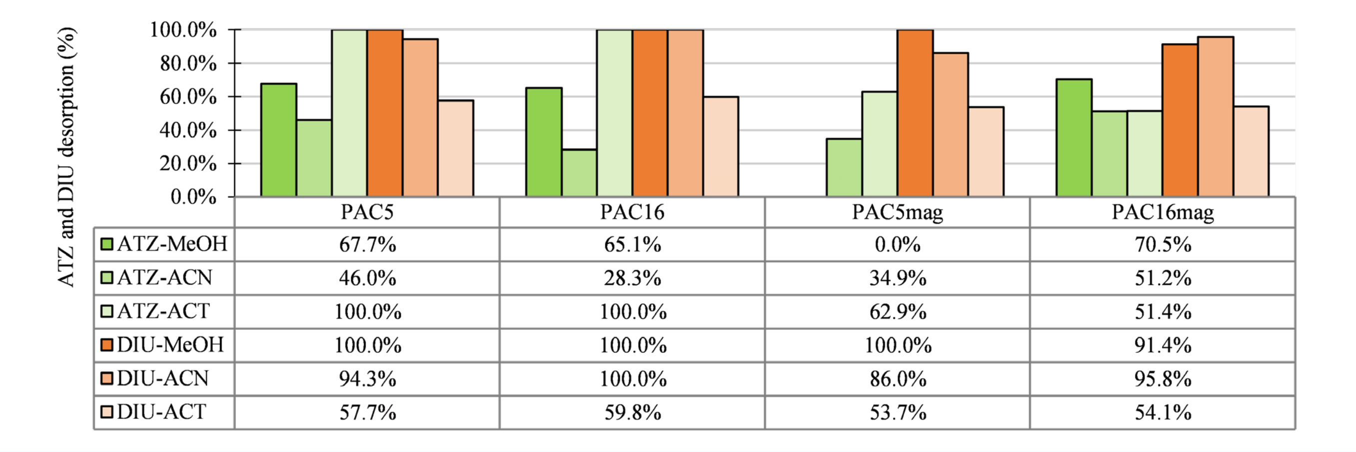
These efficiencies indicate that the use of magnets as a magnetic separation technology for PACmag from liquid could be promising for water treatment applications.

Adsorption isotherms

The adsorption isotherms, along with the determination coefficient (R^2) values and the empirically calculated parameters of the Freundlich, Langmuir, Sips, and Redlich–Peterson models, are presented in Figure 10 and Table 5.

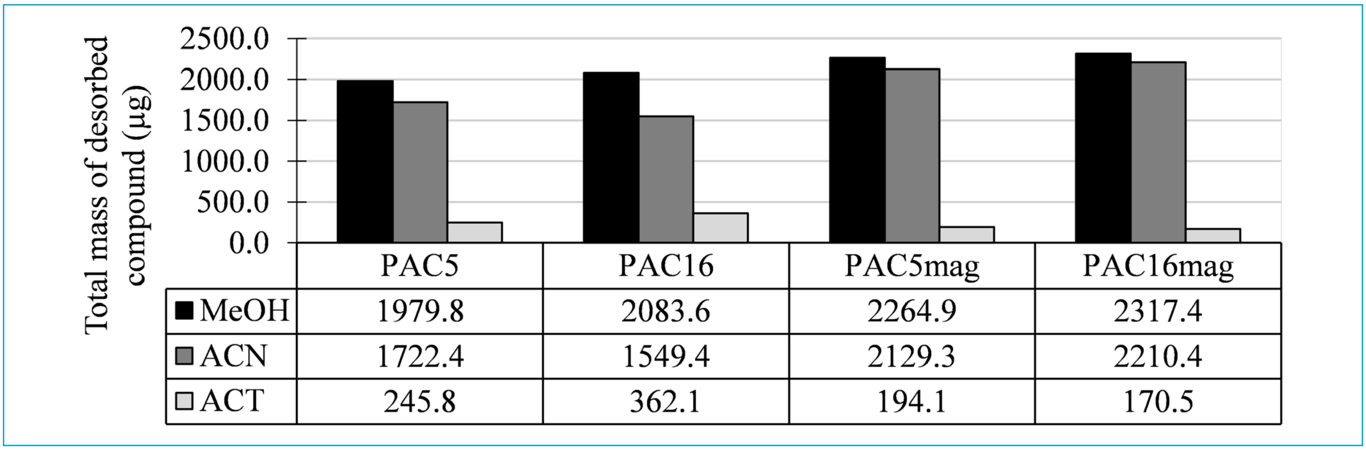
For the contaminants ATZ and SMZ, the tested models exhibited varying levels of adjustments. While the Langmuir, Freundlich, and Sips models showed R^2 values above 0.98 and 0.96, respectively, the Redlich–Peterson model demonstrated a lower adjustment for ATZ ($R^2 = 0.88$) and a moderate adjustment for SMZ ($R^2 = 0.93$). The comparison between the models for the compounds reveals that, despite the ns values approaching 1 ($ns_{ATZ} = 1.09$ and $ns_{SMZ} = 1.27$), the Sips isotherm resembles the Freundlich model, with $Ks_{ATZ} = 2.53\text{x}10^{-3}$ and $Ks_{SMZ} = 1.84\text{x}10^{-3}$, suggesting possible multilayer adsorption. This behavior may be related to the higher binding intensity observed for these compounds, as indicated by the parameters of the Freundlich isotherm, which point to a strong affinity between ATZ, SMZ, and PAC ($Kf_{ATZ} = 20.93$; $nf_{ATZ} = 1.51$ and $Kf_{SMZ} = 4.14$; $nf_{SMZ} = 1.07$). Higher nf values and lower Kf values indicate more favorable adsorption, corroborating the adsorption efficiencies observed in Figure 7. The β parameter, which reflects the hybrid behavior between the Langmuir and Freundlich models, presented values close to zero ($\beta = 1\text{x}10^{-8}$) for both ATZ and SMZ, indicating that the Redlich–Peterson model closely resembles the Freundlich model in these cases, suggesting behavior characteristic of heterogeneous systems.

Additionally, for DIU, the R^2 values range from 0.88, 0.83, 0.99, and 0.95 for Langmuir, Freundlich, Sips, and Redlich–Peterson, respectively. Although the $\beta = 2.84$ parameter in the Redlich–Peterson model suggests a tendency toward Langmuir behavior, the lower R^2 value compared to the Sips model indicates a less precise fit of the experimental data to the Redlich–Peterson model.



	PAC5	PAC16	PAC5mag	PAC16mag
🟩 ATZ-MeOH	67.7%	65.1%	0.0%	70.5%
🟩 ATZ-ACN	46.0%	28.3%	34.9%	51.2%
🟩 ATZ-ACT	100.0%	100.0%	62.9%	51.4%
🟧 DIU-MeOH	100.0%	100.0%	100.0%	91.4%
🟧 DIU-ACN	94.3%	100.0%	86.0%	95.8%
🟧 DIU-ACT	57.7%	59.8%	53.7%	54.1%

Figure 8 – Percentage of desorption of adsorbent materials concerning pesticides.



	PAC5	PAC16	PAC5mag	PAC16mag
■ MeOH	1979.8	2083.6	2264.9	2317.4
■ ACN	1722.4	1549.4	2129.3	2210.4
□ ACT	245.8	362.1	194.1	170.5

Figure 9 – Total mass of a composted compound by an adsorbent.

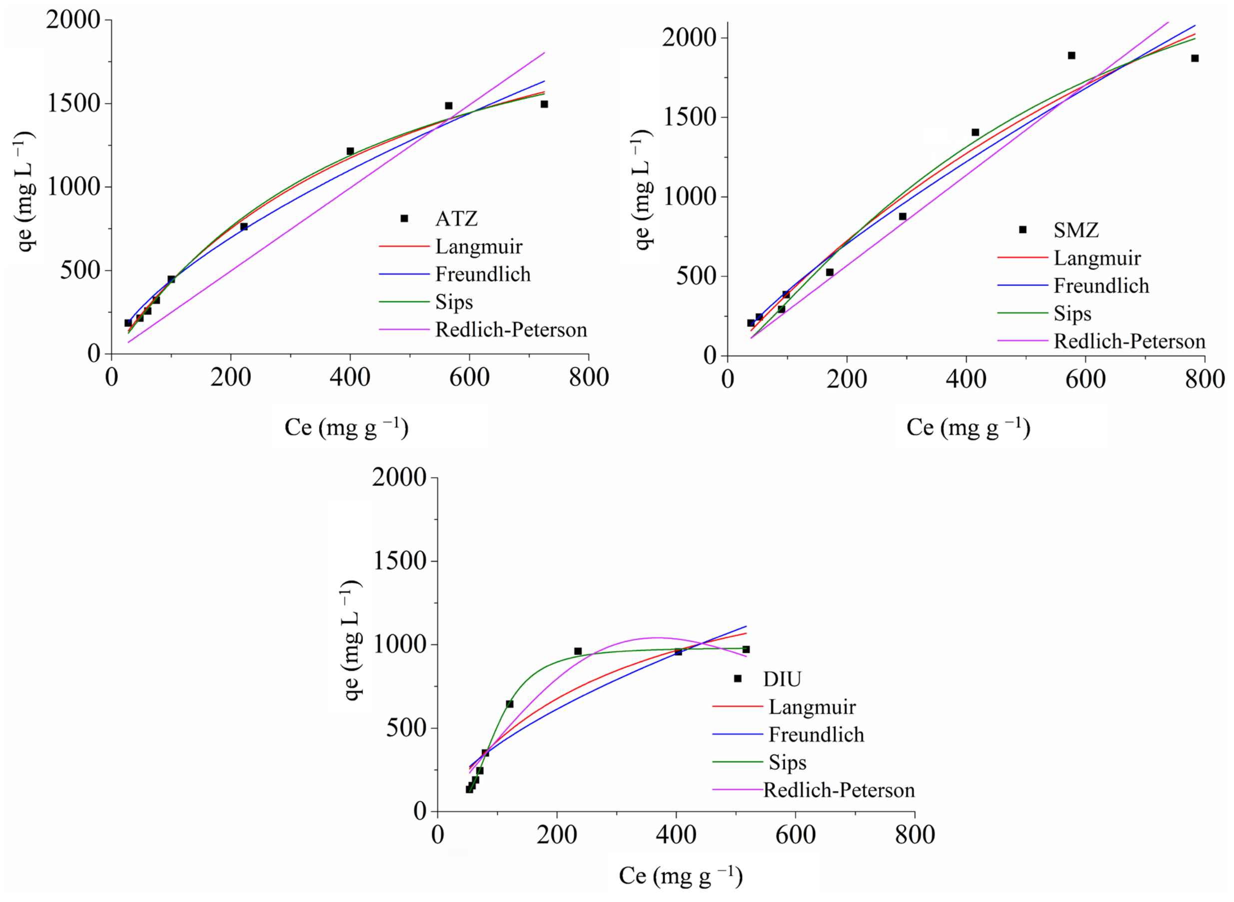


Figure 10 – Adsorption isotherms of ATZ, SMZ, and DIU for PAC16mag.

The Sips model, with $R^2 = 0.99$, demonstrates the highest predictive accuracy for DIU adsorption, and, although $R^2_{\text{Langmuir}} > R^2_{\text{Freundlich}}$, analyzing the Sips model parameters $Ks_{\text{DIU}} = 0.01$ and ns = 3.26, the equation tends to the Freundlich model. Given that most ns and nf values in the Sips and Freundlich models for the studied compounds tend to 1, this suggests relatively linear adsorption, indicating that the adsorption sites have similar energies. The Sips model combines the saturation of the Langmuir isotherm with the non-linearity of the Freundlich isotherm, providing a more suitable description of adsorption behavior in complex and heterogeneous systems (De Vargas Brião; Hashim; Chu, 2023).

The slight variation in ns suggests the presence of a mixture of high- and low-energy sites, consistent with the heterogeneity of the adsorbent surface, as observed in SEM images. This heterogeneity can be attributed to PACs, which have a porous structure with meso- and micropores of different dimensions and forms (Kumar et al., 2010), corroborating the data obtained in the characterization of micro- and mesopores (Table 4). For DIU, $\beta = 2.84$ suggests a greater contribution from high-energy sites, reinforcing the heterogeneity of the system and a distinct behavior for this compound.

Regarding equilibrium adsorption capacities (qe), it is observed that the values are consistent between ATZ and SMZ, while for DIU, the qe values are substantially lower, especially for the Sips model (1.48 mg g^{-1}). These variations observed in the empirically calculated parameters for all the models, though not aligning with expected magnitude correlations, can be attributed to the use of CPs instead of analytical standards in the study waters. The use of CPs can overestimate both the maximum adsorption capacity and the empirically calculated indices, highlighting the need for using CPs in research and technical investigations, as it is the predominant form found in natural sources.

Furthermore, the adsorption of organic compounds is influenced by the intrinsic characteristics of molecules, such as size, hydrophobicity, and the presence of functional groups that affect interactions between adsorbents and adsorbates (π–π interactions, hydrogen bonding) (Moreno-Castilla, 2004; Lladó et al., 2015; Pimenta et al., 2020).

Based on these observations, the results obtained underscore the necessity for comprehensive technical investigations into the adsorptive capacity of materials used in WTPs. The experimental conditions tested revealed that adsorption efficiency is not always directly related to the parameters obtained through mathematical models of adsorption isotherms.

Adsorption kinetics

The adsorption kinetics results for PAC16mag, adjusted to the PFO, PSO, and Elovich models, shown in Figure 11 and Table 6, revealed significant differences among ATZ, SMZ, and DIU, reflecting the unique characteristics of each compound and the heterogeneity of the adsorbent.

Overall, the Elovich model was the most robust for describing the adsorption of ATZ, SMZ, and DIU, with determination coefficients (R^2) of 0.98, 0.99, and 0.99, respectively. This model is particularly effective for heterogeneous

Table 5 – Parameters and equations obtained from the adsorption isotherms of ATZ, SMZ, and DIU for the Langmuir, Freundlich, Sips, and Redlich-Peterson models for PAC16mag.

Compound	Model	R²	Parameter	Equation
ATZ	Langmuir	0.99	qe = 138.88 qm = 2.68E+03 Kl = 1.95E-03 RL = 0.38	$Q_e = 2.68x10^3 \frac{1.95x10^{-3}Ce}{1 + 1.95x10^{-3}Ce}$
	Freundlich	0.98	qe = 189.76 Kf = 20.93 nf = 1.51	$q_e = 20.93Ce^{1}/_{1.51}$
	Sips	0.99	qe = 124.72 qm = 2360.73 Ks = 2.53E-03 ns = 1.09	$q_e = 2360.73 \frac{(2.53x10^{-3}Ce)^{1.09}}{1 + (2.53x10^{-3}Ce)^{1.09}}$
	Redlich-Peterson	0.88	qe = 69.64 KRP = 2.49 aRP = 1E-14 β = 1E-08	$qe = \frac{2.49.C_e}{1 + 1.00x10^{-14}.C_e^{1.00x10^{-08}}}$
SMZ	Langmuir	0.97	qe = 128.77 qm = 1.02E+04 Kl = 3.25E-04 RL = 0.77	$q_e = 1.02x10^4 \frac{3.25x10^{-4}Ce}{1 + 3.25x10^{-4}Ce}$
	Freundlich	0.96	qe = 128.43 Kf = 4.14 nf = 1.07	$q_e = 4.14Ce^{1}/_{1.07}$
	Sips	0.97	qe = 112.84 qm = 3.25E+03 Ks = 1.84E-03 ns = 1.27	$q_e = 3.25x10^{-3} \frac{(1.84x10^{-3}Ce)^{1.27}}{1 + (1.84x10^{-3}Ce)^{1.27}}$
	Redlich-Peterson	0.93	qe = 97.38 KRP = 2.48 aRP = 1E-14 β = 1E-08	$qe = \frac{2.48.C_e}{1 + 1.00x10^{-14}.C_e^{1.00x10^{-08}}}$
DIU	Langmuir	0.88	qe = 71.8 qm = 1683.66 Kl = 3.36E-03 RL = 0.34	$q_e = 1683.66 \frac{3.36x10^{-3}Ce}{1 + 3.36x10^{-3}Ce}$
	Freundlich	0.83	qe = 113.04 Kf = 22.56 nf = 1.6	$q_e = 22.56Ce^{1}/_{1.6}$
	Sips	0.99	qe = 1.48 qm = 982.5 Ks = 0.01 ns = 3.26	$q_e = 982.5 \frac{(0.01Ce)^{3.26}}{1 + (0.01Ce)^{3.26}}$
	Redlich-Peterson	0.95	qe = 231.87 KRP = 4.36 aRP = 2.79E-08 β = 2.84	$qe = \frac{4.36.C_e}{1 + 2.79x10^{-8}.C_e^{2.84}}$

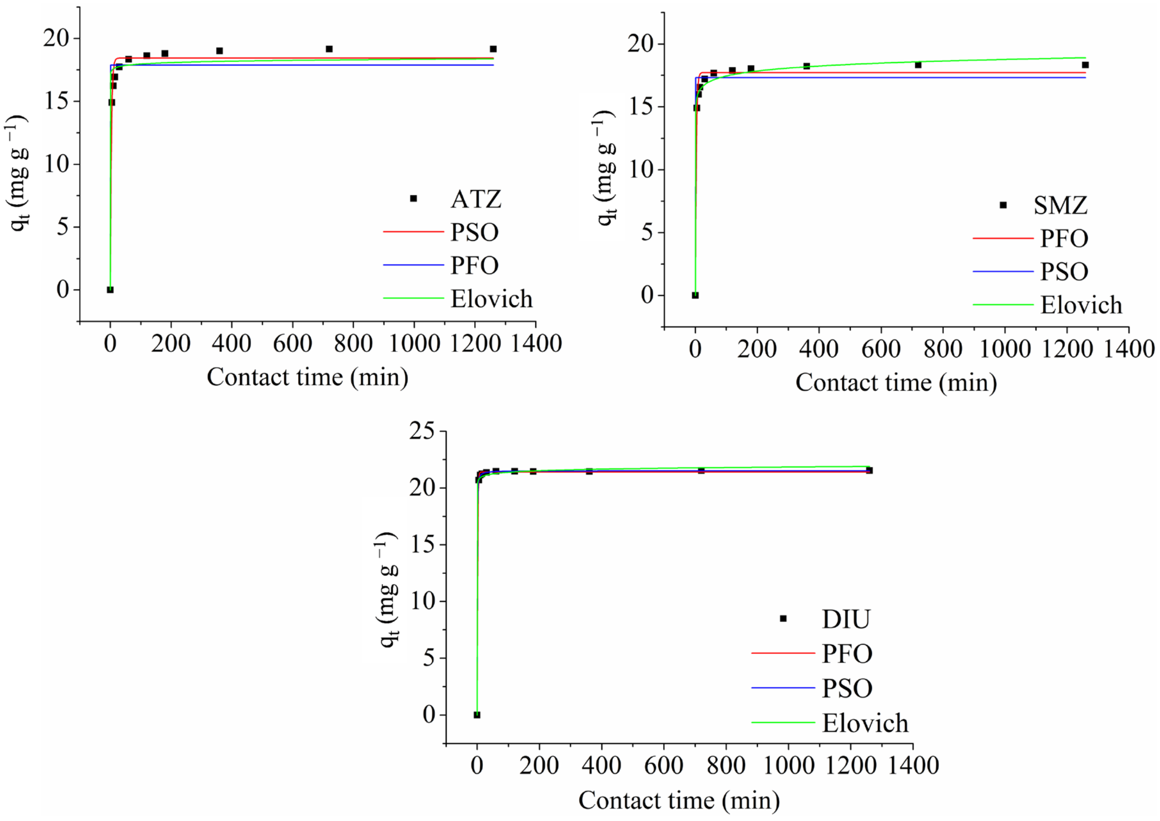


Figure 11 – Adsorption kinetics of ATZ, SMZ, and DIU for PAC16mag.

Table 6 – Parameters and equations obtained from the adsorption kinetics of ATZ, SMZ, and DIU for the pseudo-first-order, pseudo-second-order, and Elovich models for PAC16mag.

Compound	Model	R²	Parameter	Equation
ATZ	PFO	0.98	$q_e = 18.44$	$q_t = 18.44(1 - e^{-0.29t})$
			$k_1 = 0.29$	
	PSO	0.94	$q_e = 17.89$	$q_t = \frac{-3.46x10^{43}\ x\ 17.89^2 t}{1 + (-3.46x10^{43})17.89t}$
			$k_2 = -3.46x10^{43}$	
	Elovich	0.98	$\alpha = 1.11x10^{45}$	$q_t = \frac{1}{6.13} ln(1.11x10^{45}\ x\ 6.13t + 1)$
			$\beta = 6.13$	
SMZ	PFO	0.98	$q_e = 17.72$	$q_t = 17.72(1 - e^{-0.33t})$
			$k_1 = 0.33$	
	PSO	0.96	$q_e = 17.32$	$q_t = \frac{1.24x10^{45} 17.32^2 t}{1 + 1.24x17.32t}$
			$k_2 = 1.24x10^{45}$	
	Elovich	0.99	$\alpha = 1.04x10^{11}$	$q_t = \frac{1}{1.75} ln(1.04x10^{11}\ x\ 1.75t + 1)$
			$\beta = 1.75$	
DIU	PFO	0.99	$q_e = 21.41$	$q_t = 21.41(1 - e^{-0.67t})$
			$k_1 = 0.67$	
	PSO	0.99	$q_e = 21.51$	$q_t = \frac{0.24x21.51^2 t}{1 + 0.24x21.51t}$
			$k_2 = 0.24$	
	Elovich	0.99	$\alpha = 2.77x10^{43}$	$q_t = \frac{1}{4.97} ln(2.77x10^{43}\ x\ 4.97t + 1)$
			$\beta = 4.97$	

surfaces characterized by active sites of varying energies, describing processes where initial rates are high but decelerate as the active sites become saturated (Mandal; Singh; Purakayastha, 2017; Ge et al., 2019). For ATZ and SMZ, the high α values (1.11×10^{45} and 1.04×10^{11}, respectively) indicate strong initial interactions with PAC16mag, while the β values (6.13 and 1.75) reflect a slowdown in kinetics over time. For DIU, the Elovich model also showed high α (2.77×10^{43}) and β (4.97) values, consistent with the literature on pesticide adsorption onto functionalized materials, where π–π interactions, hydrogen bonding, and van der Waals forces are predominant (Ge et al., 2019; Franco et al., 2024).

The PFO model showed a good fit for ATZ and SMZ ($R^2 = 0.98$), reflecting initial control by external diffusion, a characteristic of macroporous systems. However, despite PAC16mag being predominantly microporous (Table 4), it also exhibits a significant amount of mesopores, which can facilitate the diffusion of larger molecules and enhance the adsorption of certain compounds. This aligns with studies highlighting PFO as suitable for rapid kinetics, especially in carbonaceous materials with high accessibility to active sites (Lladó et al., 2015; Coldebella et al., 2018). For DIU, the PFO model also showed a fit of $R^2 = 0.99$, with a relatively high rate constant ($k_1 = 0.67$), indicating that the initial adsorption stages are dominated by external mass transfer before intraparticle mechanisms become significant (Franco et al., 2024).

Conversely, the PSO model provided a better fit for DIU ($R^2 = 0.99$), with an equilibrium capacity (qe = 21.51 mg g^{-1}) close to the experimental value. This suggests a potential chemisorption mechanism, where specific chemical interactions at active sites play a dominant role. However, for ATZ and SMZ, the rate constant (k_2) values were inconsistent (-3.46×10^{43} for ATZ and 1.24×10^{45} for SMZ), indicating that the PSO model is inadequate to describe these systems. Previous studies corroborate this observation, noting that the PSO model's fit heavily depends on the chemical nature of the compounds and the structure of the adsorbent (Hadi et al., 2021; Franco et al., 2024).

From a practical perspective, the results indicate that PAC16mag has promising characteristics for applications in water treatment systems contaminated by pesticides. The surface heterogeneity and excellent kinetic performance for ATZ, SMZ, and DIU make it a viable alternative (Ge et al., 2019; Hadi et al., 2021). These aspects, combined with the versatility of the Elovich model for describing complex surfaces, reinforce PAC16mag's applicability in real-world scenarios, including multicomponent water systems.

Future studies could focus on optimizing environmental conditions, such as temperature, to maximize its effectiveness in large-scale systems, aligning theory and practice to advance contaminated water treatment processes (Mandal; Singh; Purakayastha, 2017; Ge et al., 2019; Franco et al., 2024).

Point of zero charge

Figure 12 presents the relationship between the initial and final pH of the solutions for the PAC16mag, indicating a pH_{PZC} value of 7.1.

The pH_{PZC} of the PAC16mag activated carbon was determined to range between pH 6.97 and 7.24, indicating that at pH 7, the carbon surface is near-neutral, with a slight tendency toward a negative charge. For aqueous solutions with pH values below the pH_{PZC}, the PAC16mag surface becomes positively charged, favoring the adsorption of anions such as chloride, which are often present in ATZ and SMZ. Conversely, at pH values above the pH_{PZC}, the surface becomes negatively charged, enhancing the adsorption of cations, including metal residues from pesticide formulations (Rodrigues et al., 2020; Wang et al., 2021).

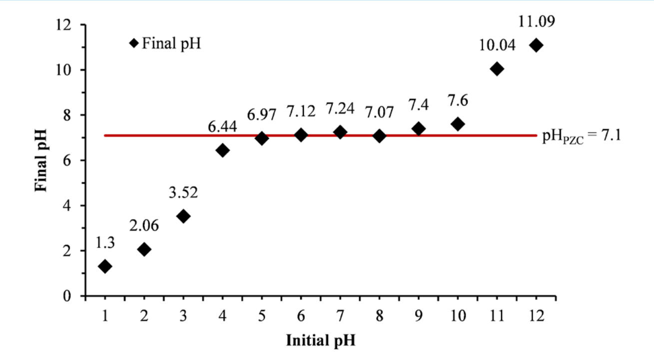


Figure 12 – PAC16mag zero charge point.

At pH 7 (Section 2.4), the ionization of the studied compounds—ATZ, SMZ, and DIU—was analyzed based on their pKa values: 1.7 for ATZ, 1.62 for SMZ, and 13.5 for DIU (Xu et al., 2018; Cusioli et al., 2019; de Souza; dos Santos, 2020; Lee; Han; Ro, 2020; Franco et al., 2024). Since the solution pH is significantly higher than the pKa values of ATZ and SMZ, these compounds predominantly exist in their deprotonated forms, carrying a negative charge. However, DIU, with a pKa of 13.5, remains largely in its protonated, neutral form at pH 7. This difference in ionization states significantly impacts their adsorption behavior.

Despite the electrostatic repulsion between the negatively charged pesticides (ATZ and SMZ) and the slightly negatively charged carbon surface, the observed adsorption order was DIU > ATZ > SMZ (Figure 7). This behavior can be explained by additional factors. First, at pH 7, the carbon surface is near-neutral, reducing the strength of repulsive interactions and allowing other mechanisms to dominate. Second, the adsorption process is likely influenced by selective interactions, such as hydrophobic effects and the specific affinity of the pesticides for functional groups on the carbon surface. DIU, being predominantly neutral, experiences minimal electrostatic interactions, potentially allowing stronger hydrophobic interactions to facilitate adsorption.

The impregnation process with magnetic nanoparticles alters surface characteristics, balancing acidic and basic functional groups, as observed in similar studies with magnetized carbonaceous materials (Rodrigues et al., 2020; Wang et al., 2021). Finally, molecular size and structure may also play a role, with DIU exhibiting a higher affinity for the adsorbent, possibly due to greater hydrophobicity or compatibility with the carbon's surface properties. These combined factors highlight the importance of the ionization state of the pesticides, the surface charge of the carbon, and the experimental pH in determining the adsorption behavior.

CONCLUSIONS

This study provides a comprehensive evaluation of the potentials and limitations of magnetized pulverized activated carbon (PAC16mag) for removing pesticides from water. The results demonstrate that PAC16mag combines high adsorption efficiency with complete desorption and recovery capabilities, making it a promising candidate for sustainable application in WTPs. The findings contribute to the field by elucidating key adsorption mechanisms, such as the role of Fe–O functional groups and hydrophobic interactions, and by integrating adsorption kinetics, isotherm models, and pH_{PZC} determination to provide a robust understanding of the adsorption process.

While these results underscore the applicability of PAC16mag, the study also identifies important limitations. The experiments were conducted using SWs, which, while controlled, do not fully account for the complexities of natural water matrices, including the presence of competing ions and dissolved organic matter. Additionally, the long-term stability of PAC16mag under repeated adsorption–desorption cycles requires further investigation. The economic viability of large-scale implementation, including solvent recovery during desorption, must also be addressed to ensure practicality.

Despite these challenges, this study advances the development of magnetic adsorbents and their application in water treatment, providing a foundation for future research aimed at optimizing performance under real-world conditions. The insights gained here contribute significantly to the ongoing efforts to develop efficient, cost-effective, and sustainable technologies for addressing pesticide contamination in water sources.

AUTHORS' CONTRIBUTIONS

Avila, F. D.: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. Pimenta, J. A. A.: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Visualization, Writing – review & editing. Nogueira, H. P.: Investigation, Methodology, Visualization, Writing – review & editing. Rodrigues, L. A.: Investigation, Methodology, Writing – review & editing. Araki, K.: Investigation, Methodology, Resources, Funding acquisition. Kuroda, E. K.: Conceptualization, Formal Analysis, Funding acquisition, Methodology, Resources, Supervision, Writing – review & editing.

DATA AVAILABILITY STATEMENT

The datasets generated and/or analyzed during the current study are available from the corresponding author upon reasonable request.

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